



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 04:04 PM BST

PDB ID : 6D6A  
Title : The structure of ligand binding domain of LasR in complex with TP-1 homolog, compound 10  
Authors : Dong, S.H.; Nair, S.K.  
Deposited on : 2018-04-20  
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

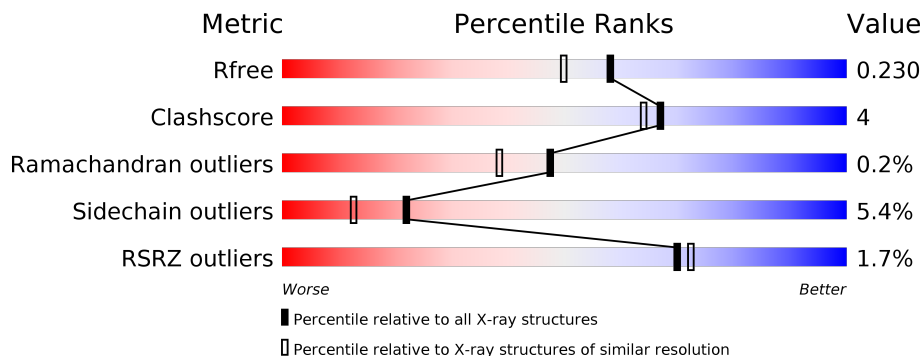
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



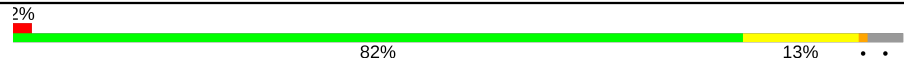

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	170	 89% 8% .
1	B	170	 87% 9% ..
1	C	170	 84% 14% .
1	D	170	 85% 11% ..
1	E	170	 88% 9% .
1	F	170	 88% 9% ...

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Mol	Chain	Length	Quality of chain
1	G	170	 2% 82% 13% . .
1	H	170	 2% 82% 14% . .

## 2 Entry composition

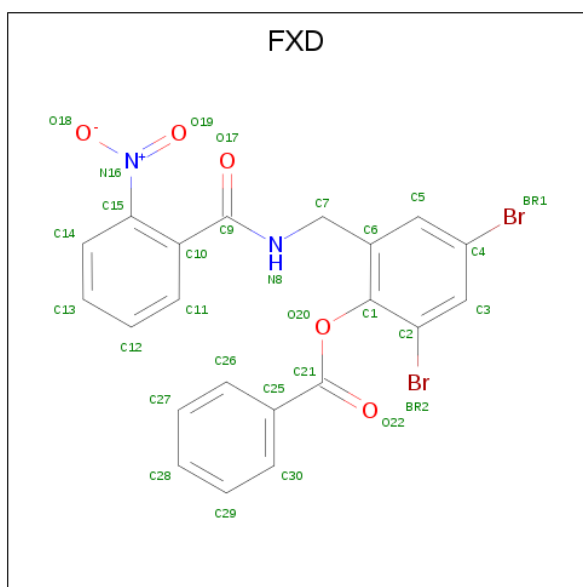
There are 3 unique types of molecules in this entry. The entry contains 11361 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Transcriptional activator protein LasR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	166	1311	841	218	247	5	0	2	0
1	B	166	1310	841	218	246	5	0	2	0
1	C	166	1311	841	218	247	5	0	2	0
1	D	165	1302	835	217	245	5	0	2	0
1	E	165	1304	835	217	247	5	0	2	0
1	F	167	1315	844	219	247	5	0	2	0
1	G	164	1294	829	216	244	5	0	2	0
1	H	166	1311	841	218	247	5	0	2	0

- Molecule 2 is 2,4-dibromo-6-{{(2-nitrobenzene-1-carbonyl)amino}methyl}phenyl benzoate (three-letter code: FXD) (formula: C<sub>21</sub>H<sub>14</sub>Br<sub>2</sub>N<sub>2</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	Br	C	N	O		
2	A	1	Total 30	Br 2	C 21	N 2	O 5	0	0
2	B	1	Total 30	Br 2	C 21	N 2	O 5	0	0
2	C	1	Total 30	Br 2	C 21	N 2	O 5	0	0
2	D	1	Total 30	Br 2	C 21	N 2	O 5	0	0
2	E	1	Total 30	Br 2	C 21	N 2	O 5	0	0
2	F	1	Total 30	Br 2	C 21	N 2	O 5	0	0
2	G	1	Total 30	Br 2	C 21	N 2	O 5	0	0
2	H	1	Total 30	Br 2	C 21	N 2	O 5	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	75	Total 75	O 75	0	0
3	B	75	Total 75	O 75	0	0
3	C	85	Total 85	O 85	0	0
3	D	67	Total 67	O 67	0	0

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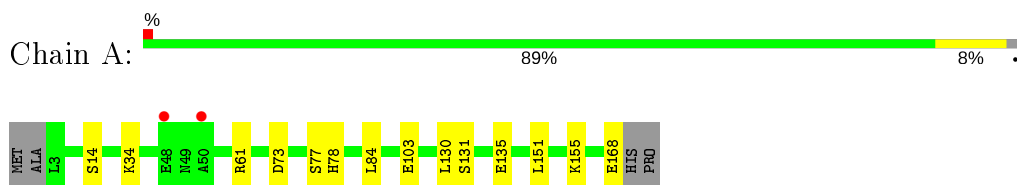
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
3	E	87	Total O 87 87	0	0
3	F	105	Total O 105 105	0	0
3	G	85	Total O 85 85	0	0
3	H	84	Total O 84 84	0	0

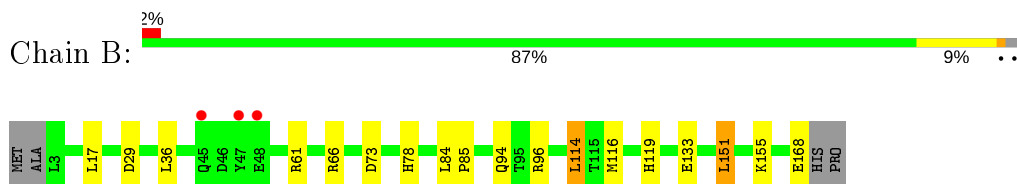
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

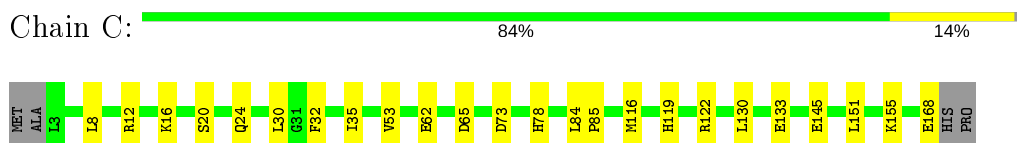
- Molecule 1: Transcriptional activator protein LasR



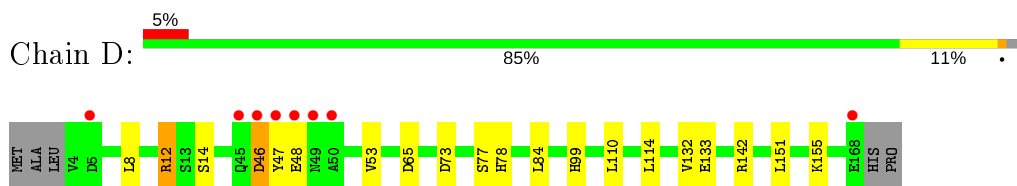
- Molecule 1: Transcriptional activator protein LasR



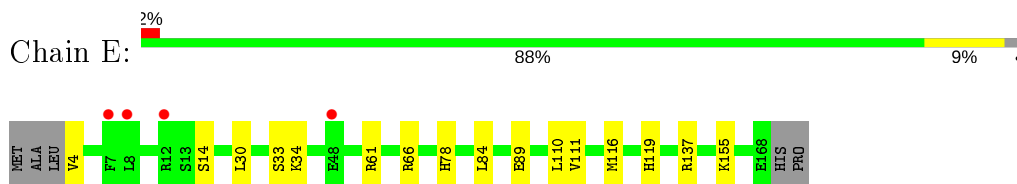
- Molecule 1: Transcriptional activator protein LasR



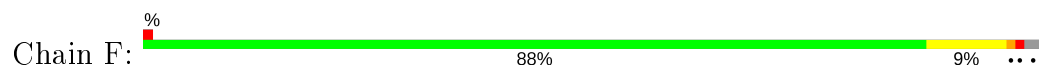
- Molecule 1: Transcriptional activator protein LasR



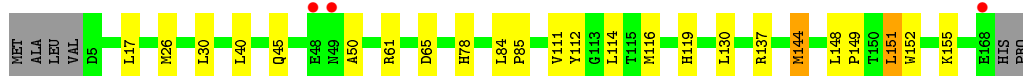
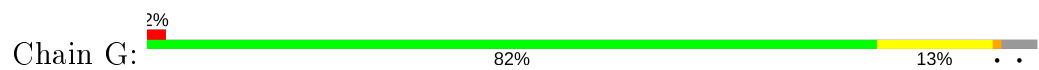
- Molecule 1: Transcriptional activator protein LasR



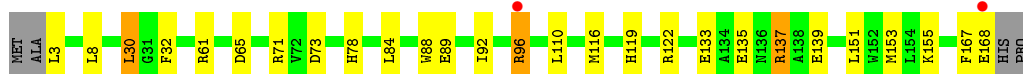
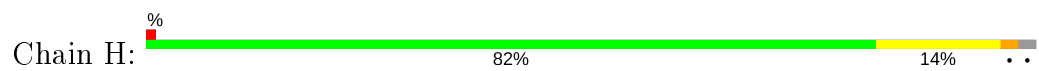
- Molecule 1: Transcriptional activator protein LasR



- Molecule 1: Transcriptional activator protein LasR



- Molecule 1: Transcriptional activator protein LasR





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.28Å 84.45Å 156.20Å 90.00° 95.71° 90.00°	Depositor
Resolution (Å)	38.86 – 1.90 38.86 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.6 (38.86-1.90) 97.6 (38.86-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.92 (at 1.89Å)	Xtrriage
Refinement program	REFMAC 5.8.0189	Depositor
R, $R_{free}$	0.179 , 0.224 0.188 , 0.230	Depositor DCC
$R_{free}$ test set	5401 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.9	Xtrriage
Anisotropy	0.596	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 49.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11361	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.61 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.1344e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: FXD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.92	1/1350 (0.1%)	0.91	1/1829 (0.1%)
1	B	0.89	0/1344	0.97	5/1821 (0.3%)
1	C	0.93	1/1350 (0.1%)	0.93	2/1829 (0.1%)
1	D	0.91	0/1336	0.97	4/1810 (0.2%)
1	E	0.92	0/1348	0.89	1/1826 (0.1%)
1	F	0.94	0/1349	1.04	6/1828 (0.3%)
1	G	0.89	0/1338	0.92	1/1812 (0.1%)
1	H	0.91	0/1350	0.97	7/1829 (0.4%)
All	All	0.91	2/10765 (0.0%)	0.95	27/14584 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	62	GLU	CD-OE1	5.61	1.31	1.25
1	A	77	SER	CB-OG	-5.04	1.35	1.42

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	73	ASP	CB-CG-OD2	-9.55	109.70	118.30
1	H	122	ARG	NE-CZ-NH1	9.45	125.03	120.30
1	F	12	ARG	NE-CZ-NH2	-8.24	116.18	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	12	ARG	NE-CZ-NH1	7.91	124.25	120.30
1	B	73	ASP	CB-CG-OD1	7.53	125.08	118.30
1	F	142	ARG	NE-CZ-NH1	7.53	124.06	120.30
1	F	61	ARG	NE-CZ-NH2	-7.25	116.68	120.30
1	C	73	ASP	CB-CG-OD2	-7.01	111.99	118.30
1	H	137	ARG	NE-CZ-NH2	6.85	123.72	120.30
1	B	73	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	H	73	ASP	CB-CG-OD2	-6.75	112.22	118.30
1	D	73	ASP	CB-CG-OD1	6.25	123.93	118.30
1	H	137	ARG	NE-CZ-NH1	-6.16	117.22	120.30
1	C	73	ASP	CB-CG-OD1	6.13	123.82	118.30
1	F	71	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	B	61	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	H	65	ASP	CB-CG-OD1	5.60	123.34	118.30
1	B	96	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	F	144	MET	CG-SD-CE	5.44	108.91	100.20
1	H	30	LEU	CB-CG-CD1	5.33	120.07	111.00
1	B	29	ASP	CB-CG-OD1	5.31	123.08	118.30
1	E	89	GLU	OE1-CD-OE2	5.23	129.57	123.30
1	A	73	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	H	122	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	G	144	MET	CG-SD-CE	5.11	108.37	100.20
1	D	77	SER	N-CA-CB	5.09	118.14	110.50
1	D	142	ARG	NE-CZ-NH1	5.06	122.83	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	167	PHE	Peptide

## 5.2 Too-close contacts [\(i\)](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1311	0	1264	8	0
1	B	1310	0	1261	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1311	0	1264	14	0
1	D	1302	0	1250	5	0
1	E	1304	0	1256	6	0
1	F	1315	0	1266	10	0
1	G	1294	0	1245	13	0
1	H	1311	0	1264	14	0
2	A	30	0	0	0	0
2	B	30	0	0	1	0
2	C	30	0	0	0	0
2	D	30	0	0	1	0
2	E	30	0	0	2	0
2	F	30	0	0	1	0
2	G	30	0	0	0	0
2	H	30	0	0	2	0
3	A	75	0	0	4	1
3	B	75	0	0	5	0
3	C	85	0	0	3	3
3	D	67	0	0	1	0
3	E	87	0	0	3	0
3	F	105	0	0	6	3
3	G	85	0	0	2	1
3	H	84	0	0	5	0
All	All	11361	0	10070	81	4

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (81) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:104:GLU:CD	3:F:401:HOH:O	1.83	1.15
1:C:35:ILE:HG22	1:C:130:LEU:HD23	1.76	0.67
1:B:94:GLN:HG2	3:B:433:HOH:O	1.94	0.67
1:C:20[A]:SER:OG	1:C:24:GLN:NE2	2.28	0.67
1:C:35:ILE:CG2	1:C:130:LEU:HD23	2.24	0.67
1:E:78:HIS:HE1	1:E:84:LEU:O	1.79	0.65
1:H:88:TRP:O	1:H:137:ARG:NH1	2.31	0.63
1:G:78:HIS:HE1	1:G:84:LEU:O	1.81	0.63
1:A:78:HIS:HE1	1:A:84:LEU:O	1.84	0.60
1:B:78:HIS:HE1	1:B:84:LEU:O	1.85	0.60
1:C:16:LYS:O	1:C:20[B]:SER:OG	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:78:HIS:HE1	1:D:84:LEU:O	1.86	0.59
1:C:20[B]:SER:HB3	1:C:53:VAL:HG13	1.84	0.59
1:B:78:HIS:HD2	3:B:472:HOH:O	1.86	0.58
1:F:78:HIS:HE1	1:F:84:LEU:O	1.86	0.58
1:H:168:GLU:CD	3:H:401:HOH:O	2.42	0.58
1:B:94:GLN:HG2	3:B:469:HOH:O	2.03	0.57
1:F:142:ARG:HD3	3:F:475:HOH:O	2.03	0.57
1:B:119:HIS:HD2	3:B:428:HOH:O	1.89	0.56
1:C:78:HIS:HE1	1:C:84:LEU:O	1.89	0.56
1:F:119:HIS:HD2	3:F:442:HOH:O	1.88	0.56
1:D:110:LEU:HD13	2:D:300:FXD:O18	2.06	0.56
1:F:85:PRO:HB3	1:F:116:MET:SD	2.47	0.55
1:H:78:HIS:HE1	1:H:84:LEU:O	1.91	0.54
1:C:32:PHE:CE1	1:C:151:LEU:HD21	2.44	0.52
1:H:119:HIS:HD2	3:H:437:HOH:O	1.90	0.52
1:A:61:ARG:NH1	3:A:404:HOH:O	2.41	0.52
1:G:119:HIS:HD2	3:G:416:HOH:O	1.93	0.52
1:H:96:ARG:N	1:H:96:ARG:CD	2.73	0.52
1:H:135:GLU:HG2	1:H:139:GLU:OE1	2.09	0.52
1:F:104:GLU:OE2	3:F:401:HOH:O	2.11	0.51
1:A:61:ARG:CZ	3:A:404:HOH:O	2.58	0.51
1:C:85:PRO:HB3	1:C:116:MET:SD	2.51	0.51
2:E:300:FXD:C21	2:E:300:FXD:BR2	3.14	0.51
1:E:119:HIS:HD2	3:E:438:HOH:O	1.94	0.51
1:D:8:LEU:O	1:D:12:ARG:HG3	2.12	0.49
1:G:152:TRP:CD2	1:H:153:MET:HG2	2.47	0.49
1:H:96:ARG:N	1:H:96:ARG:HD3	2.26	0.49
1:E:66:ARG:HD3	3:E:402:HOH:O	2.13	0.49
1:G:114:LEU:HD11	1:G:151:LEU:HD12	1.93	0.49
1:A:135:GLU:HG3	1:G:112:TYR:OH	2.13	0.48
1:H:168:GLU:OE2	3:H:401:HOH:O	2.20	0.48
1:G:114:LEU:HD11	1:G:151:LEU:CD1	2.43	0.48
2:H:300:FXD:C21	2:H:300:FXD:BR2	3.17	0.48
1:F:12:ARG:HH11	1:F:12:ARG:CG	2.27	0.47
1:D:78:HIS:HD2	3:D:463:HOH:O	1.98	0.46
1:B:85:PRO:HB3	1:B:116:MET:SD	2.56	0.46
1:E:61:ARG:CZ	3:E:446:HOH:O	2.62	0.46
1:C:12:ARG:HD3	3:C:473:HOH:O	2.16	0.46
1:A:78:HIS:HD2	3:A:474:HOH:O	1.98	0.45
1:B:114:LEU:HD11	1:B:151:LEU:CD1	2.46	0.45
1:A:34:LYS:HE3	3:A:425:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:LEU:HD11	1:B:151:LEU:HD13	1.99	0.45
1:G:26:MET:O	1:G:30:LEU:HD13	2.17	0.45
1:E:33:SER:O	1:E:34:LYS:HD3	2.17	0.44
1:G:130:LEU:HD12	1:G:130:LEU:N	2.32	0.44
1:H:168:GLU:C	3:H:429:HOH:O	2.55	0.44
1:A:135:GLU:OE1	1:G:137:ARG:NH2	2.51	0.44
1:G:85:PRO:HB3	1:G:116:MET:SD	2.57	0.44
2:B:300:FXD:C21	2:B:300:FXD:BR2	3.20	0.44
1:D:46:ASP:O	1:D:48:GLU:N	2.51	0.43
1:G:40:LEU:HD23	1:G:50:ALA:HA	2.00	0.43
1:C:35:ILE:HG21	1:C:130:LEU:HD23	2.00	0.43
1:C:30:LEU:HD23	1:C:151:LEU:HD23	1.99	0.43
1:F:104:GLU:OE1	3:F:401:HOH:O	2.17	0.43
1:H:110:LEU:HD13	2:H:300:FXD:O18	2.19	0.42
1:B:17:LEU:HD13	1:B:17:LEU:C	2.39	0.42
1:C:30:LEU:CD2	1:C:151:LEU:HD23	2.50	0.42
2:F:300:FXD:C21	2:F:300:FXD:BR2	3.23	0.42
1:F:32:PHE:CE2	1:F:151:LEU:HD21	2.55	0.42
1:H:61:ARG:NH1	3:H:404:HOH:O	2.45	0.41
1:A:130:LEU:HD12	1:A:130:LEU:N	2.34	0.41
1:H:32:PHE:CZ	1:H:151:LEU:HD11	2.55	0.41
1:G:148:LEU:HB3	1:G:149:PRO:HD3	2.02	0.41
1:H:89:GLU:O	1:H:92:ILE:HG12	2.20	0.41
1:B:36:LEU:HD22	3:B:459:HOH:O	2.20	0.41
1:F:104:GLU:CB	3:F:401:HOH:O	2.69	0.41
1:C:119:HIS:HD2	3:C:433:HOH:O	2.02	0.41
1:E:110:LEU:HD13	2:E:300:FXD:O18	2.21	0.41
1:C:12:ARG:CD	3:C:473:HOH:O	2.68	0.40
1:G:61:ARG:CD	3:G:414:HOH:O	2.68	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:402:HOH:O	3:F:477:HOH:O[1_655]	2.08	0.12
3:A:439:HOH:O	3:G:483:HOH:O[2_755]	2.11	0.09
3:C:406:HOH:O	3:F:475:HOH:O[1_655]	2.15	0.05
3:C:424:HOH:O	3:F:475:HOH:O[1_655]	2.16	0.04

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	165/170 (97%)	161 (98%)	4 (2%)	0	100	100
1	B	164/170 (96%)	160 (98%)	4 (2%)	0	100	100
1	C	165/170 (97%)	162 (98%)	3 (2%)	0	100	100
1	D	163/170 (96%)	159 (98%)	2 (1%)	2 (1%)	13	4
1	E	165/170 (97%)	165 (100%)	0	0	100	100
1	F	165/170 (97%)	163 (99%)	2 (1%)	0	100	100
1	G	164/170 (96%)	162 (99%)	2 (1%)	0	100	100
1	H	165/170 (97%)	164 (99%)	1 (1%)	0	100	100
All	All	1316/1360 (97%)	1296 (98%)	18 (1%)	2 (0%)	47	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	46	ASP
1	D	47	TYR

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	136/138 (99%)	129 (95%)	7 (5%)	24	14
1	B	135/138 (98%)	129 (96%)	6 (4%)	28	19
1	C	136/138 (99%)	129 (95%)	7 (5%)	24	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	134/138 (97%)	124 (92%)	10 (8%)	13	5
1	E	136/138 (99%)	129 (95%)	7 (5%)	24	14
1	F	135/138 (98%)	128 (95%)	7 (5%)	23	14
1	G	134/138 (97%)	127 (95%)	7 (5%)	23	14
1	H	136/138 (99%)	128 (94%)	8 (6%)	19	10
All	All	1082/1104 (98%)	1023 (94%)	59 (6%)	22	12

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	SER
1	A	103	GLU
1	A	131[A]	SER
1	A	131[B]	SER
1	A	151	LEU
1	A	155	LYS
1	A	168	GLU
1	B	66	ARG
1	B	114	LEU
1	B	133	GLU
1	B	151	LEU
1	B	155	LYS
1	B	168	GLU
1	C	8	LEU
1	C	65	ASP
1	C	122	ARG
1	C	133	GLU
1	C	145	GLU
1	C	155	LYS
1	C	168	GLU
1	D	12	ARG
1	D	14	SER
1	D	53	VAL
1	D	65	ASP
1	D	99	HIS
1	D	114	LEU
1	D	132	VAL
1	D	133	GLU
1	D	151	LEU
1	D	155	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	4	VAL
1	E	14	SER
1	E	30	LEU
1	E	111	VAL
1	E	116	MET
1	E	137	ARG
1	E	155	LYS
1	F	8	LEU
1	F	12	ARG
1	F	17	LEU
1	F	111	VAL
1	F	133	GLU
1	F	144	MET
1	F	155	LYS
1	G	17	LEU
1	G	45	GLN
1	G	65	ASP
1	G	111	VAL
1	G	144	MET
1	G	151	LEU
1	G	155	LYS
1	H	3	LEU
1	H	8	LEU
1	H	30	LEU
1	H	71	ARG
1	H	96	ARG
1	H	116	MET
1	H	133	GLU
1	H	155	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	78	HIS
1	A	99	HIS
1	A	119	HIS
1	B	24	GLN
1	B	49	ASN
1	B	78	HIS
1	B	119	HIS
1	C	24	GLN
1	C	45	GLN

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Mol	Chain	Res	Type
1	C	49	ASN
1	C	78	HIS
1	C	119	HIS
1	D	24	GLN
1	D	45	GLN
1	D	49	ASN
1	D	78	HIS
1	D	119	HIS
1	E	78	HIS
1	E	119	HIS
1	F	49	ASN
1	F	78	HIS
1	F	119	HIS
1	G	78	HIS
1	G	119	HIS
1	H	24	GLN
1	H	78	HIS
1	H	119	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FXD	H	300	-	31,32,32	2.07	5 (16%)	40,44,44	1.71	9 (22%)
2	FXD	B	300	-	31,32,32	1.98	6 (19%)	40,44,44	1.44	10 (25%)
2	FXD	E	300	-	31,32,32	1.84	6 (19%)	40,44,44	1.65	9 (22%)
2	FXD	G	300	-	31,32,32	2.05	4 (12%)	40,44,44	1.74	9 (22%)
2	FXD	D	300	-	31,32,32	2.08	5 (16%)	40,44,44	1.78	10 (25%)
2	FXD	A	300	-	31,32,32	1.89	4 (12%)	40,44,44	1.71	8 (20%)
2	FXD	F	300	-	31,32,32	2.11	5 (16%)	40,44,44	1.71	8 (20%)
2	FXD	C	300	-	31,32,32	1.89	6 (19%)	40,44,44	1.48	6 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FXD	H	300	-	-	4/19/21/21	0/3/3/3
2	FXD	B	300	-	-	7/19/21/21	0/3/3/3
2	FXD	E	300	-	-	3/19/21/21	0/3/3/3
2	FXD	G	300	-	-	5/19/21/21	0/3/3/3
2	FXD	D	300	-	-	5/19/21/21	0/3/3/3
2	FXD	A	300	-	-	7/19/21/21	0/3/3/3
2	FXD	F	300	-	-	4/19/21/21	0/3/3/3
2	FXD	C	300	-	-	5/19/21/21	0/3/3/3

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	300	FXD	O19-N16	9.41	1.38	1.22
2	G	300	FXD	O19-N16	9.18	1.38	1.22
2	H	300	FXD	O19-N16	9.18	1.38	1.22
2	F	300	FXD	O19-N16	8.56	1.37	1.22
2	B	300	FXD	O19-N16	8.44	1.37	1.22
2	A	300	FXD	O19-N16	8.16	1.36	1.22
2	C	300	FXD	O19-N16	7.20	1.35	1.22
2	E	300	FXD	O19-N16	7.03	1.34	1.22
2	F	300	FXD	C9-N8	-4.34	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	300	FXD	C15-N16	-4.14	1.38	1.45
2	D	300	FXD	C9-N8	-4.03	1.25	1.33
2	A	300	FXD	C15-N16	-3.81	1.38	1.45
2	C	300	FXD	C15-N16	-3.81	1.38	1.45
2	G	300	FXD	C15-N16	-3.51	1.39	1.45
2	E	300	FXD	O20-C21	3.07	1.45	1.35
2	H	300	FXD	C15-N16	-3.07	1.40	1.45
2	E	300	FXD	C9-N8	-2.95	1.27	1.33
2	C	300	FXD	O20-C21	2.94	1.45	1.35
2	G	300	FXD	C9-N8	-2.88	1.27	1.33
2	C	300	FXD	O20-C1	-2.86	1.35	1.41
2	D	300	FXD	C15-N16	-2.79	1.40	1.45
2	H	300	FXD	O20-C1	-2.78	1.35	1.41
2	C	300	FXD	C9-N8	-2.76	1.27	1.33
2	B	300	FXD	C9-N8	-2.50	1.28	1.33
2	B	300	FXD	C15-N16	-2.48	1.41	1.45
2	H	300	FXD	C9-N8	-2.46	1.28	1.33
2	E	300	FXD	O20-C1	-2.41	1.36	1.41
2	G	300	FXD	O20-C21	2.39	1.43	1.35
2	E	300	FXD	C15-N16	-2.38	1.41	1.45
2	F	300	FXD	O20-C1	-2.36	1.36	1.41
2	B	300	FXD	BR2-C2	-2.27	1.84	1.89
2	H	300	FXD	C5-C6	2.22	1.43	1.39
2	D	300	FXD	C7-N8	-2.19	1.41	1.46
2	E	300	FXD	O17-C9	2.11	1.27	1.23
2	A	300	FXD	O20-C1	-2.10	1.36	1.41
2	A	300	FXD	C9-N8	-2.06	1.29	1.33
2	B	300	FXD	O20-C21	2.05	1.42	1.35
2	B	300	FXD	O20-C1	-2.05	1.37	1.41
2	D	300	FXD	O20-C21	2.05	1.42	1.35
2	F	300	FXD	O20-C21	2.01	1.42	1.35
2	C	300	FXD	O17-C9	2.00	1.27	1.23

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	300	FXD	O20-C21-C25	4.86	122.01	111.63
2	D	300	FXD	BR1-C4-C5	-4.79	112.61	119.27
2	H	300	FXD	O17-C9-C10	-4.56	112.68	121.01
2	F	300	FXD	C10-C9-N8	4.49	126.19	117.36
2	A	300	FXD	O17-C9-C10	-4.41	112.95	121.01
2	E	300	FXD	C26-C25-C30	4.25	124.64	118.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	300	FXD	C6-C1-C2	4.24	122.33	116.94
2	G	300	FXD	O17-C9-C10	-4.16	113.41	121.01
2	H	300	FXD	O20-C21-C25	4.14	120.47	111.63
2	E	300	FXD	C27-C26-C25	-4.13	115.45	120.34
2	G	300	FXD	C10-C9-N8	4.07	125.36	117.36
2	D	300	FXD	O20-C21-C25	4.03	120.25	111.63
2	F	300	FXD	O20-C21-C25	3.97	120.11	111.63
2	A	300	FXD	C6-C1-C2	3.88	121.88	116.94
2	A	300	FXD	O20-C21-C25	3.88	119.92	111.63
2	F	300	FXD	O17-C9-C10	-3.80	114.08	121.01
2	D	300	FXD	BR1-C4-C3	3.76	124.50	119.27
2	F	300	FXD	C6-C1-C2	3.73	121.69	116.94
2	E	300	FXD	C6-C1-C2	3.49	121.38	116.94
2	B	300	FXD	O20-C21-C25	3.49	119.08	111.63
2	C	300	FXD	O17-C9-C10	-3.47	114.66	121.01
2	D	300	FXD	C7-N8-C9	3.34	129.70	121.81
2	H	300	FXD	C6-C1-C2	3.31	121.15	116.94
2	H	300	FXD	C10-C9-N8	3.15	123.54	117.36
2	G	300	FXD	C7-N8-C9	3.06	129.05	121.81
2	B	300	FXD	O17-C9-C10	-2.99	115.55	121.01
2	H	300	FXD	BR1-C4-C5	-2.98	115.12	119.27
2	A	300	FXD	C27-C26-C25	-2.92	116.88	120.34
2	H	300	FXD	C26-C25-C30	2.89	122.71	118.59
2	D	300	FXD	C6-C1-C2	2.83	120.54	116.94
2	G	300	FXD	C6-C1-C2	2.82	120.52	116.94
2	C	300	FXD	BR2-C2-C1	2.76	122.54	118.51
2	A	300	FXD	C14-C15-N16	2.76	119.42	116.47
2	A	300	FXD	O20-C21-O22	-2.74	117.29	123.14
2	B	300	FXD	C6-C1-C2	2.73	120.41	116.94
2	F	300	FXD	BR1-C4-C5	-2.66	115.56	119.27
2	C	300	FXD	C14-C15-N16	2.59	119.25	116.47
2	G	300	FXD	BR1-C4-C5	-2.58	115.68	119.27
2	D	300	FXD	O17-C9-C10	-2.57	116.32	121.01
2	C	300	FXD	O20-C21-C25	2.50	116.98	111.63
2	E	300	FXD	C12-C13-C14	-2.50	116.38	120.19
2	B	300	FXD	O20-C21-O22	-2.46	117.88	123.14
2	C	300	FXD	C3-C2-C1	-2.39	118.11	122.54
2	D	300	FXD	C26-C25-C30	2.37	121.96	118.59
2	A	300	FXD	C10-C9-N8	2.36	122.00	117.36
2	F	300	FXD	C1-O20-C21	2.36	123.66	117.50
2	E	300	FXD	O20-C21-C25	2.34	116.63	111.63
2	A	300	FXD	C26-C25-C30	2.34	121.91	118.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	300	FXD	BR1-C4-C5	-2.29	116.08	119.27
2	H	300	FXD	BR1-C4-C3	2.28	122.44	119.27
2	F	300	FXD	O20-C21-O22	-2.27	118.28	123.14
2	E	300	FXD	O17-C9-C10	-2.27	116.86	121.01
2	D	300	FXD	C6-C7-N8	2.27	117.82	113.03
2	E	300	FXD	BR1-C4-C5	-2.22	116.17	119.27
2	E	300	FXD	C30-C25-C21	-2.22	115.38	120.40
2	G	300	FXD	BR1-C4-C3	2.20	122.33	119.27
2	G	300	FXD	O20-C21-O22	-2.20	118.44	123.14
2	H	300	FXD	C27-C26-C25	-2.17	117.78	120.34
2	E	300	FXD	O20-C1-C6	2.16	121.98	118.43
2	D	300	FXD	C1-O20-C21	2.13	123.07	117.50
2	B	300	FXD	C14-C15-N16	2.13	118.75	116.47
2	B	300	FXD	C26-C25-C30	2.10	121.58	118.59
2	B	300	FXD	C7-N8-C9	2.09	126.75	121.81
2	B	300	FXD	BR1-C4-C3	2.08	122.16	119.27
2	F	300	FXD	C7-N8-C9	2.06	126.68	121.81
2	H	300	FXD	O20-C21-O22	-2.02	118.82	123.14
2	G	300	FXD	C13-C14-C15	2.01	122.04	118.61
2	B	300	FXD	C1-O20-C21	2.01	122.76	117.50
2	D	300	FXD	C27-C26-C25	-2.01	117.97	120.34

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	300	FXD	O20-C21-C25-C30
2	D	300	FXD	O20-C21-C25-C26
2	D	300	FXD	O22-C21-C25-C30
2	D	300	FXD	O22-C21-C25-C26
2	B	300	FXD	O22-C21-C25-C30
2	E	300	FXD	C1-C6-C7-N8
2	B	300	FXD	O20-C21-C25-C30
2	B	300	FXD	O22-C21-C25-C26
2	B	300	FXD	O20-C21-C25-C26
2	A	300	FXD	C1-C6-C7-N8
2	A	300	FXD	O20-C21-C25-C30
2	A	300	FXD	O20-C21-C25-C26
2	H	300	FXD	C1-C6-C7-N8
2	B	300	FXD	C1-C6-C7-N8
2	F	300	FXD	C1-C6-C7-N8
2	C	300	FXD	C1-C6-C7-N8

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Mol	Chain	Res	Type	Atoms
2	C	300	FXD	O20-C21-C25-C26
2	A	300	FXD	O22-C21-C25-C30
2	F	300	FXD	O20-C21-C25-C30
2	A	300	FXD	O22-C21-C25-C26
2	G	300	FXD	C1-C6-C7-N8
2	E	300	FXD	C14-C15-N16-O19
2	A	300	FXD	C14-C15-N16-O19
2	A	300	FXD	C5-C6-C7-N8
2	H	300	FXD	C2-C1-O20-C21
2	F	300	FXD	C5-C6-C7-N8
2	C	300	FXD	O20-C21-C25-C30
2	H	300	FXD	C5-C6-C7-N8
2	E	300	FXD	C5-C6-C7-N8
2	C	300	FXD	C5-C6-C7-N8
2	H	300	FXD	C14-C15-N16-O19
2	D	300	FXD	C14-C15-N16-O19
2	G	300	FXD	O20-C21-C25-C30
2	F	300	FXD	O20-C21-C25-C26
2	G	300	FXD	C14-C15-N16-O19
2	C	300	FXD	O22-C21-C25-C26
2	G	300	FXD	C2-C1-O20-C21
2	B	300	FXD	C15-C10-C9-O17
2	G	300	FXD	O20-C21-C25-C26
2	B	300	FXD	C5-C6-C7-N8

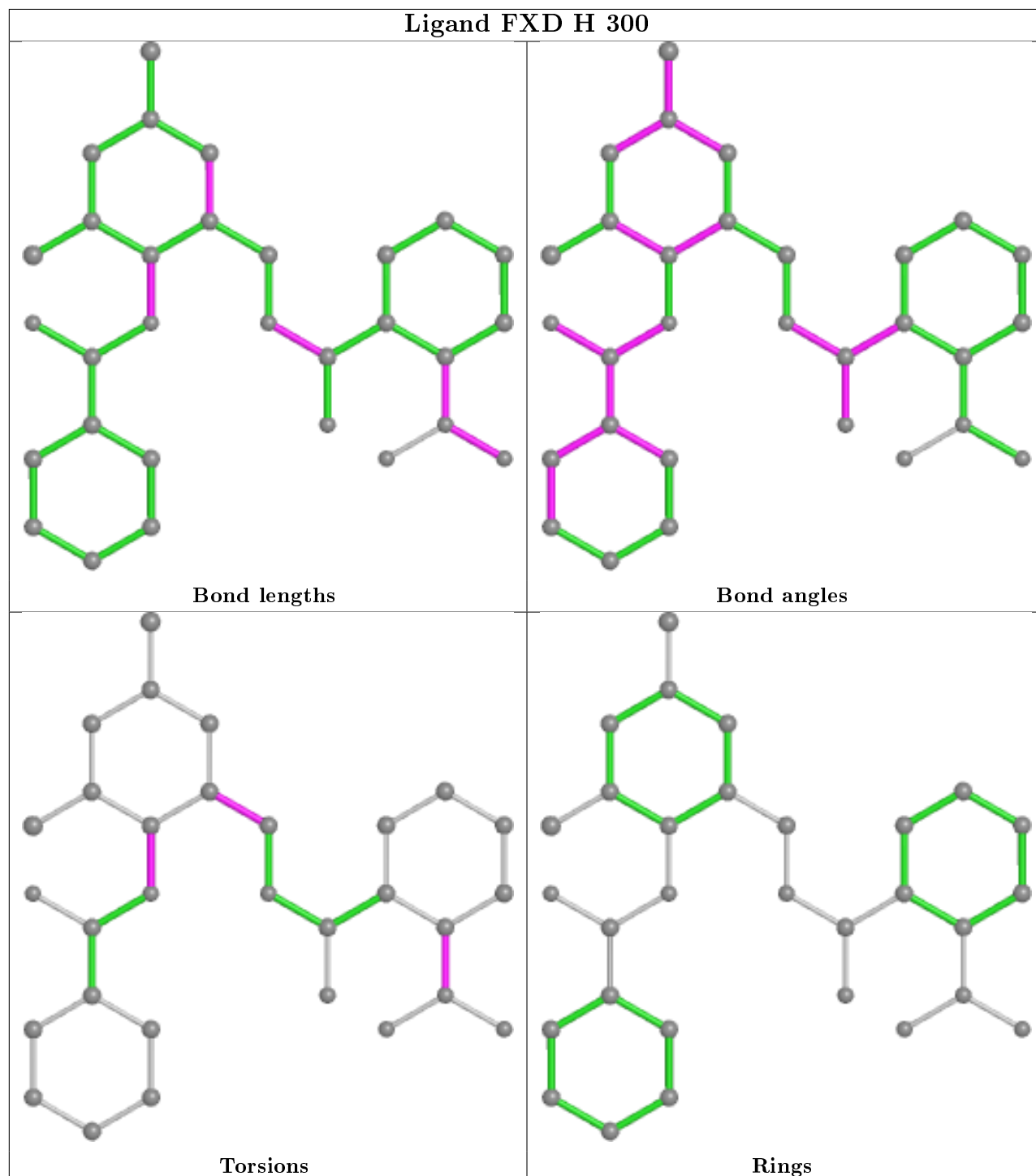
There are no ring outliers.

5 monomers are involved in 7 short contacts:

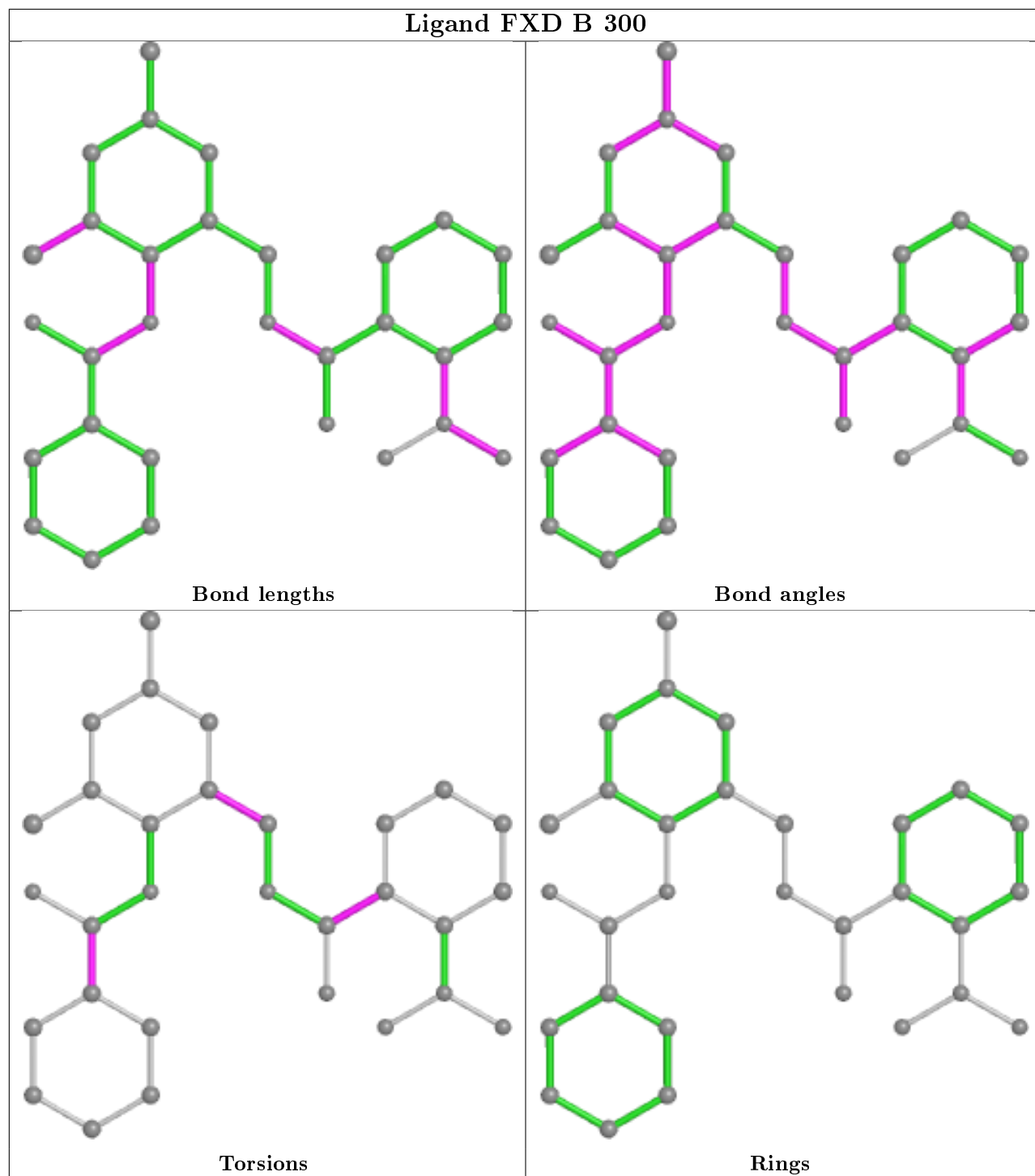
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	300	FXD	2	0
2	B	300	FXD	1	0
2	E	300	FXD	2	0
2	D	300	FXD	1	0
2	F	300	FXD	1	0

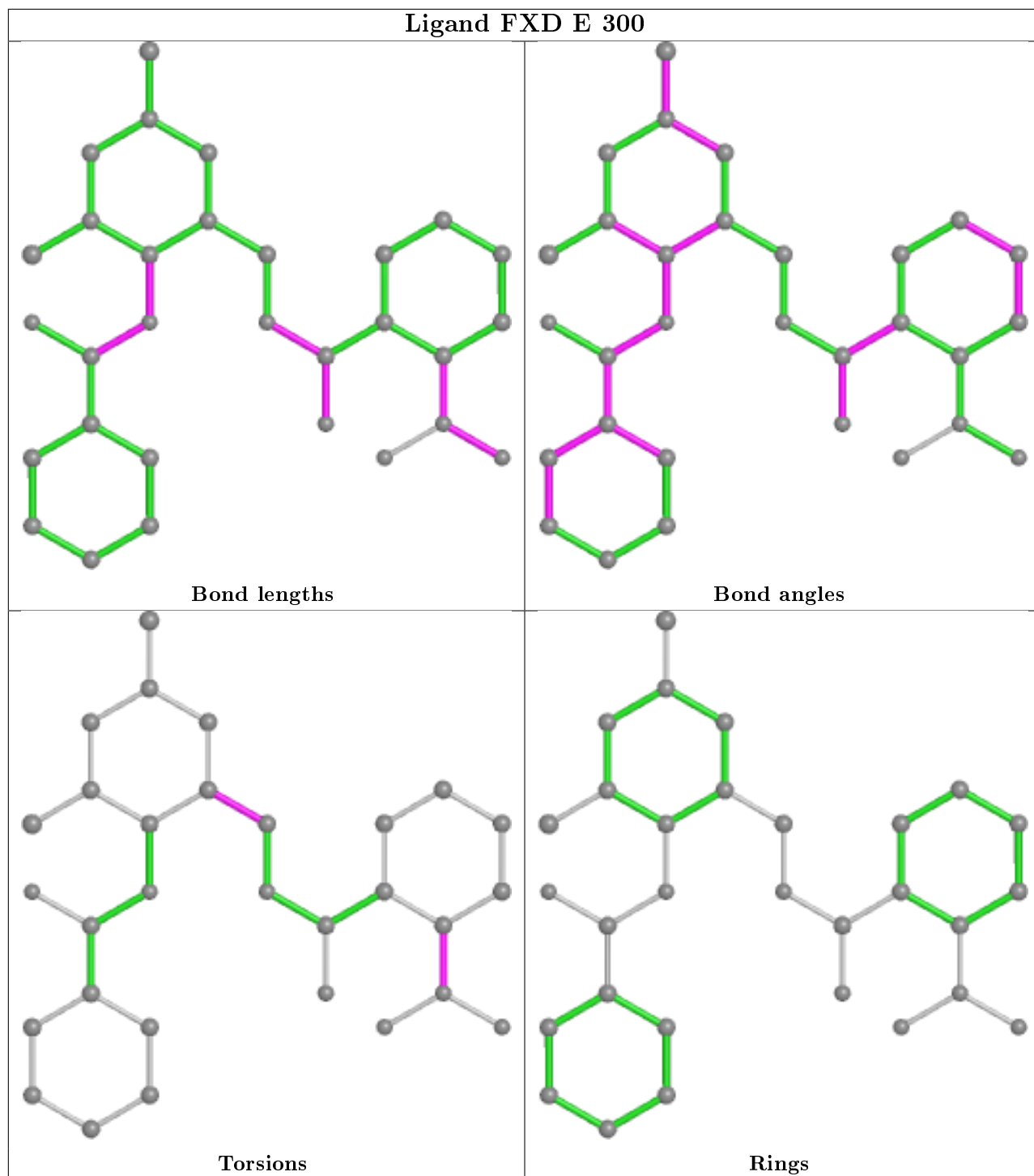
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

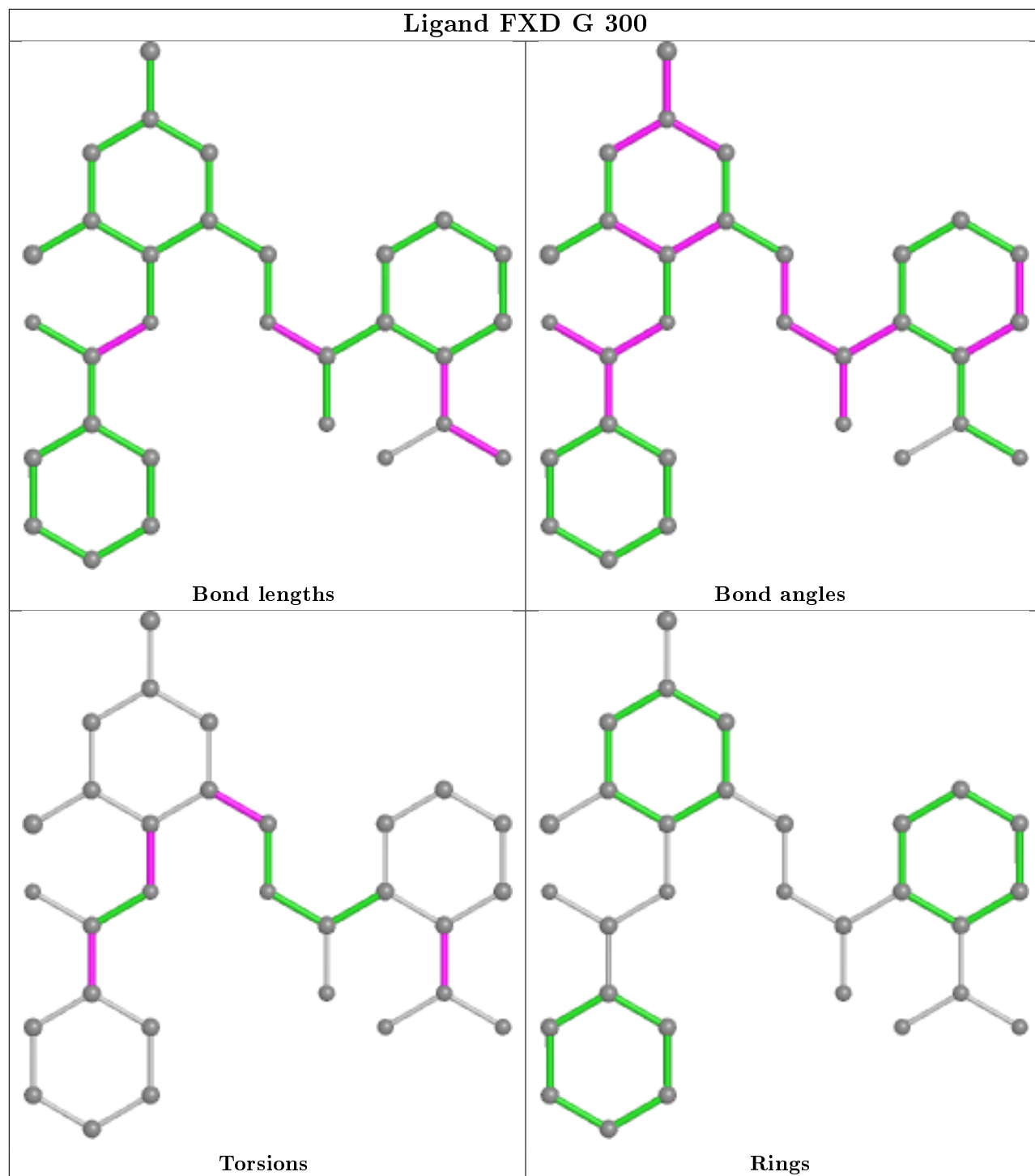
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

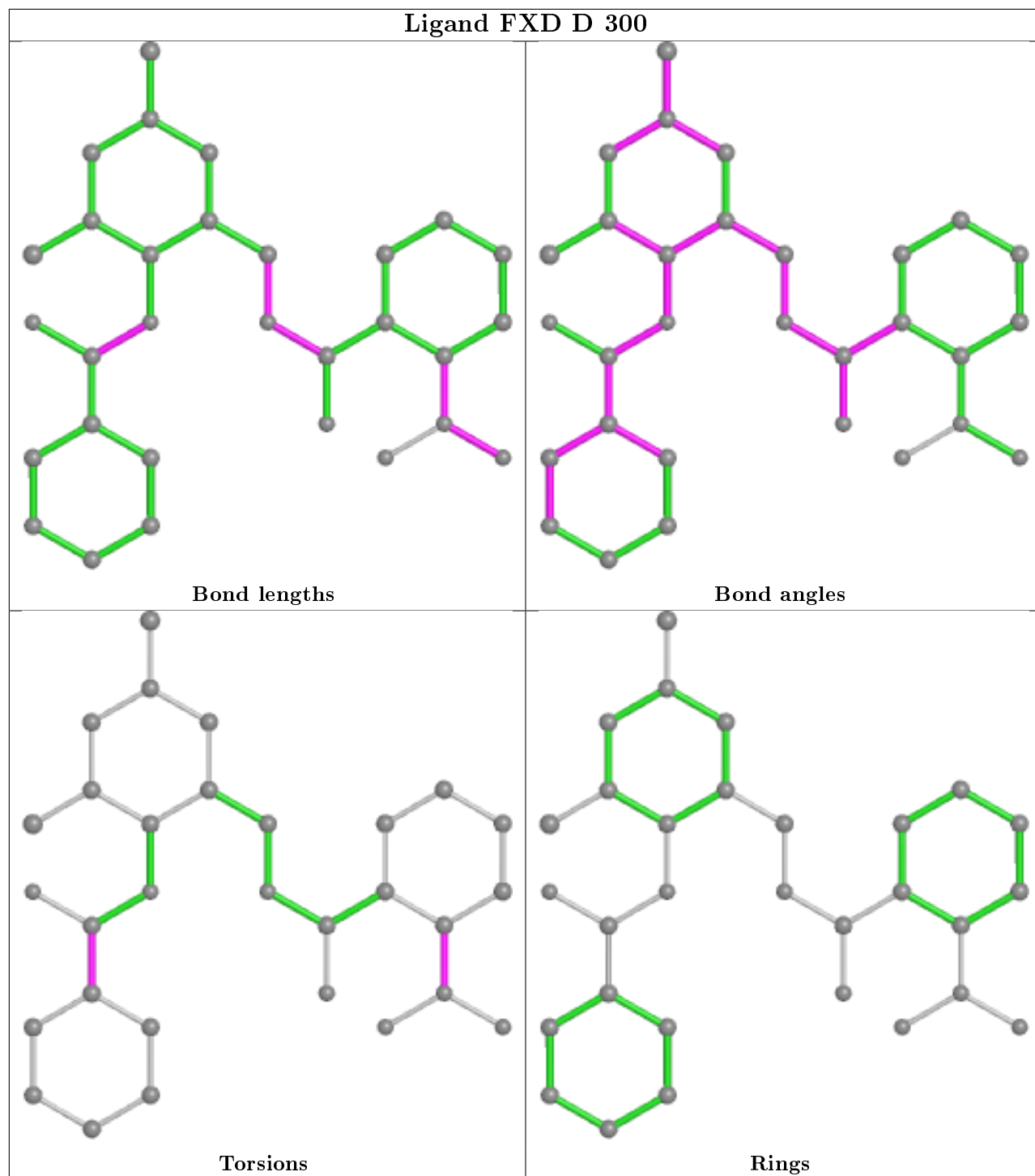


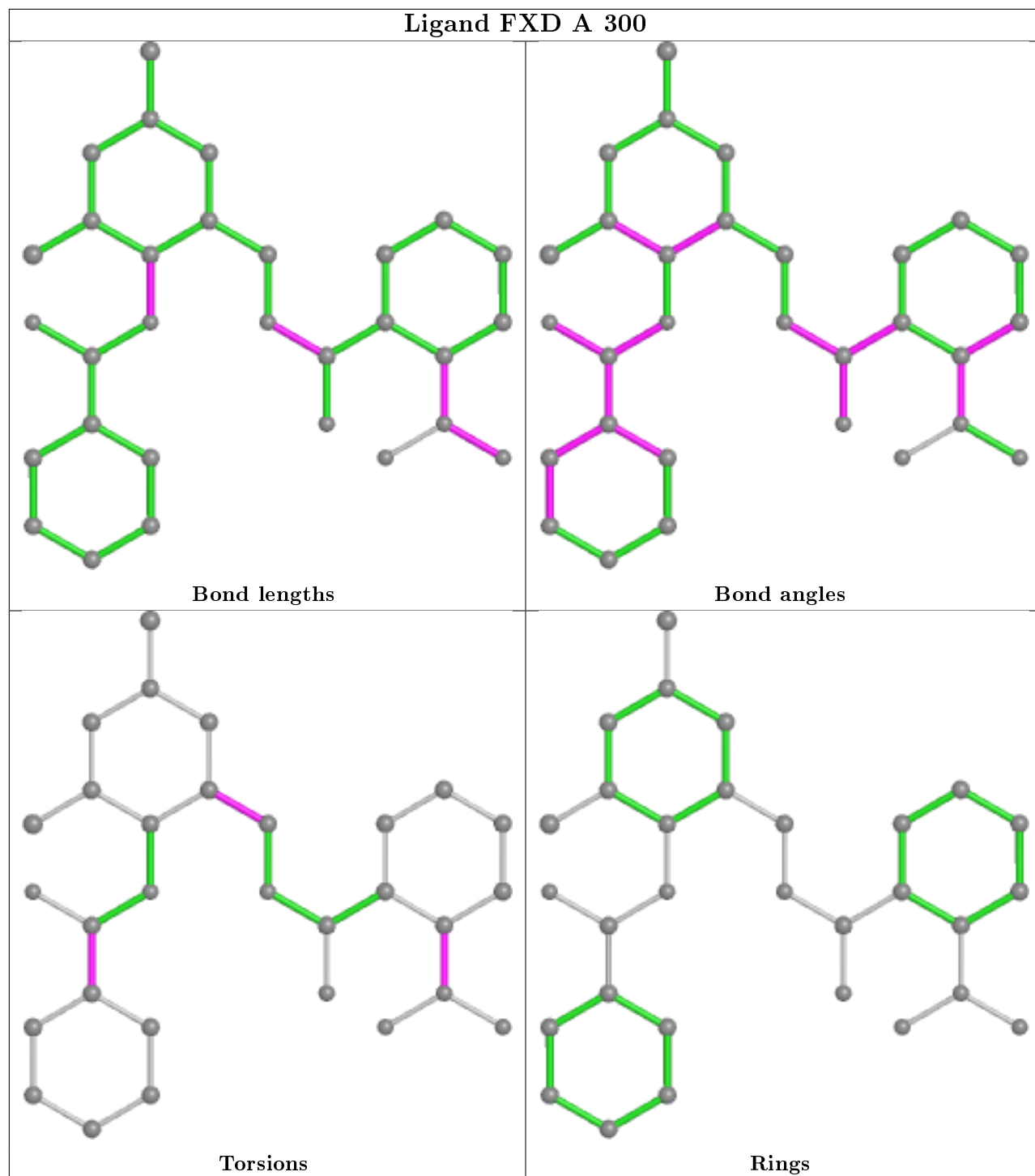


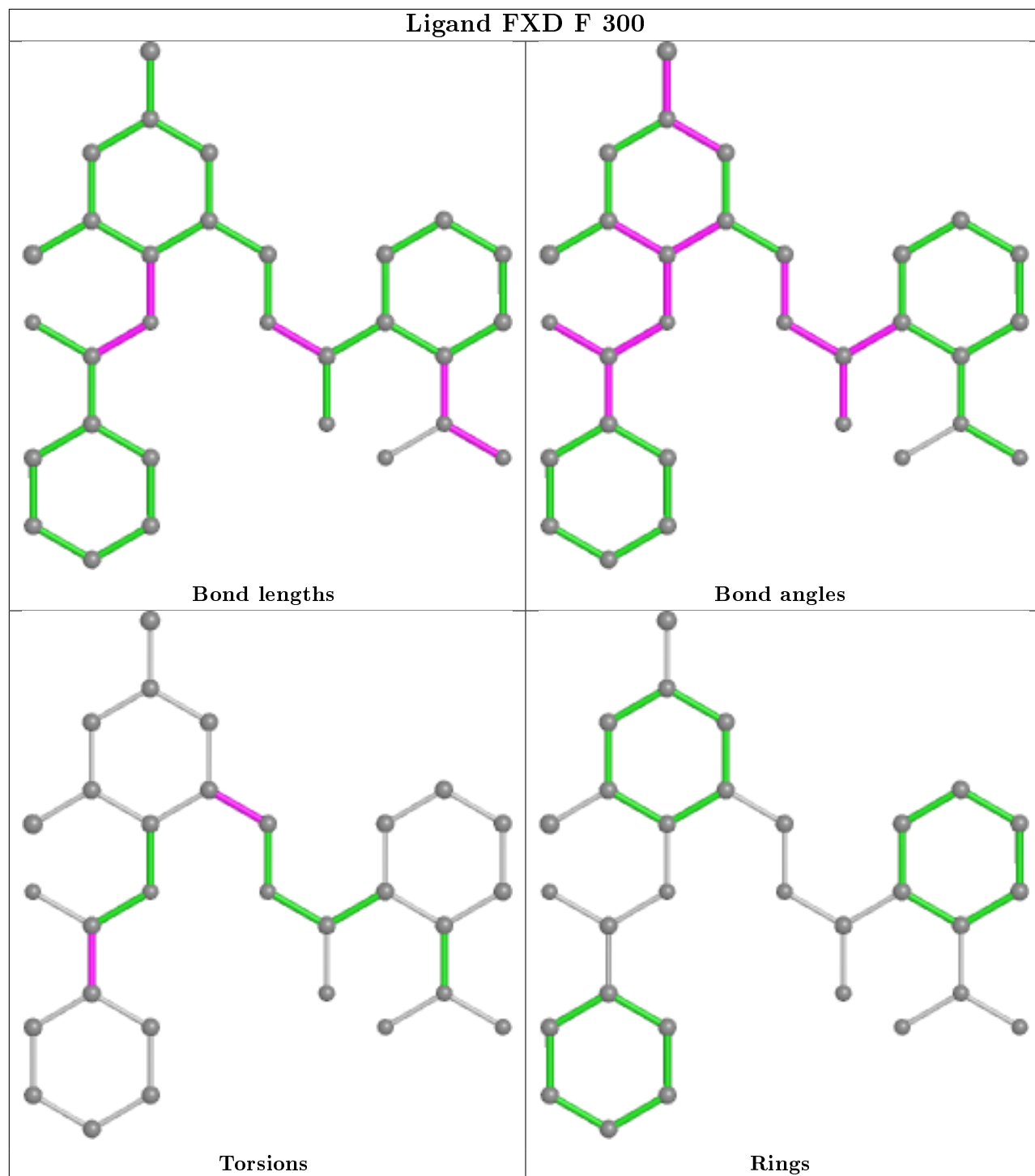


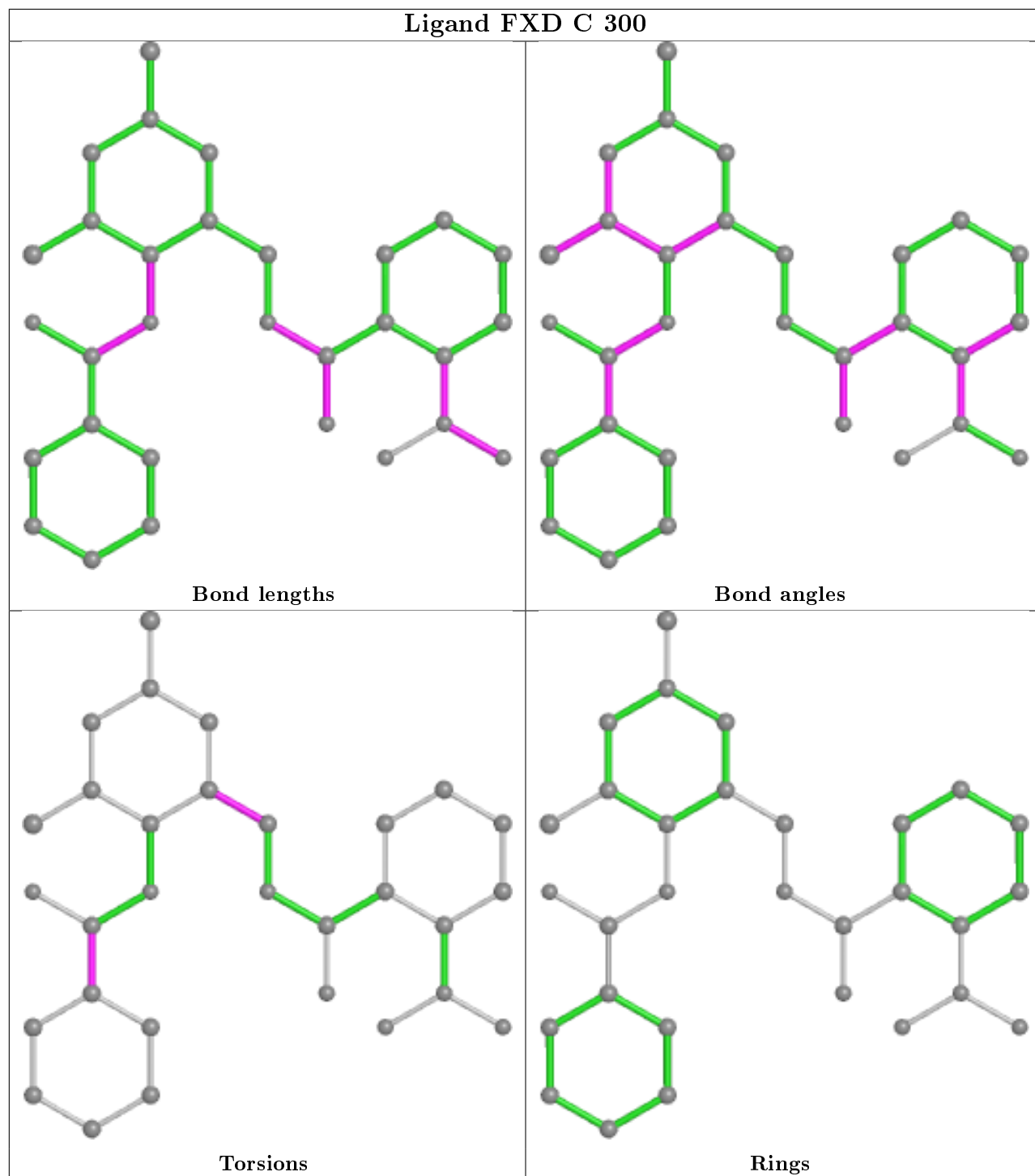












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	166/170 (97%)	-0.28	2 (1%) 79 81	16, 26, 46, 72	0
1	B	166/170 (97%)	-0.22	3 (1%) 68 71	17, 26, 53, 82	0
1	C	166/170 (97%)	-0.43	0 100 100	17, 23, 43, 56	0
1	D	165/170 (97%)	-0.14	8 (4%) 30 33	17, 26, 57, 83	0
1	E	165/170 (97%)	-0.28	4 (2%) 59 62	15, 24, 46, 68	0
1	F	167/170 (98%)	-0.35	1 (0%) 89 90	14, 21, 38, 67	0
1	G	164/170 (96%)	-0.28	3 (1%) 68 71	15, 25, 46, 77	0
1	H	166/170 (97%)	-0.22	2 (1%) 79 81	16, 25, 48, 69	0
All	All	1325/1360 (97%)	-0.27	23 (1%) 70 72	14, 25, 48, 83	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	45	GLN	5.0
1	B	48	GLU	4.4
1	G	168	GLU	4.2
1	D	47	TYR	4.0
1	A	48	GLU	3.6
1	B	47	TYR	3.4
1	D	48	GLU	3.3
1	H	96	ARG	3.1
1	D	49	ASN	3.0
1	F	168	GLU	3.0
1	G	48	GLU	2.8
1	D	168	GLU	2.7
1	E	12	ARG	2.5
1	E	7	PHE	2.4
1	E	48	GLU	2.4
1	D	50	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	45	GLN	2.3
1	E	8	LEU	2.3
1	G	49	ASN	2.2
1	D	46	ASP	2.2
1	H	168	GLU	2.1
1	A	50	ALA	2.1
1	D	5	ASP	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

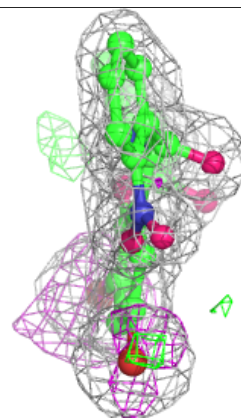
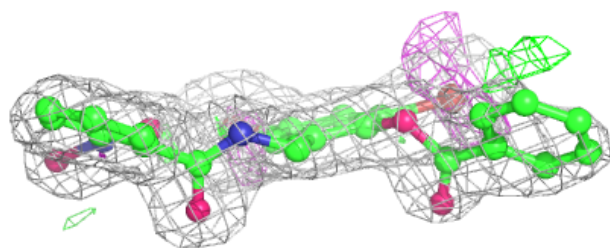
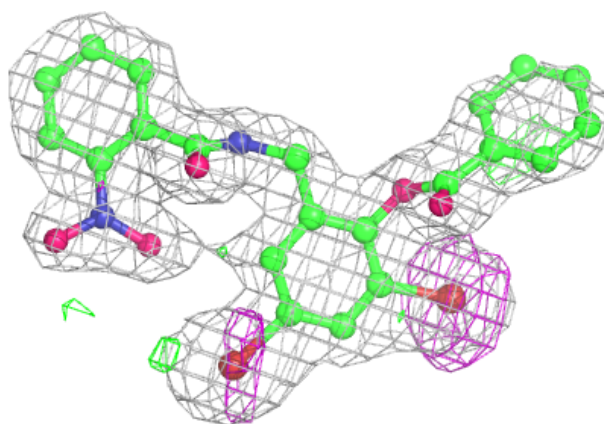
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	FXD	B	300	30/30	0.98	0.09	21,27,46,54	0
2	FXD	D	300	30/30	0.98	0.09	20,28,48,50	0
2	FXD	E	300	30/30	0.99	0.08	19,23,29,33	0
2	FXD	G	300	30/30	0.99	0.08	19,25,30,36	0
2	FXD	H	300	30/30	0.99	0.07	19,23,27,33	0
2	FXD	A	300	30/30	0.99	0.08	21,24,34,36	0
2	FXD	F	300	30/30	0.99	0.08	16,19,24,29	0
2	FXD	C	300	30/30	0.99	0.08	15,22,26,32	0

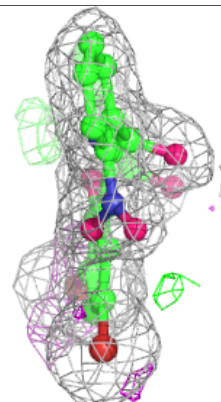
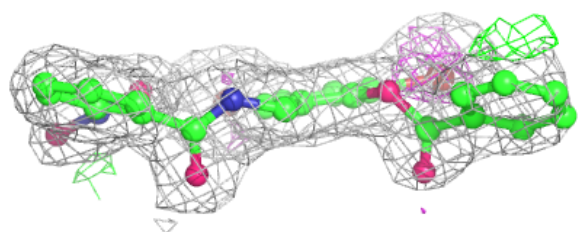
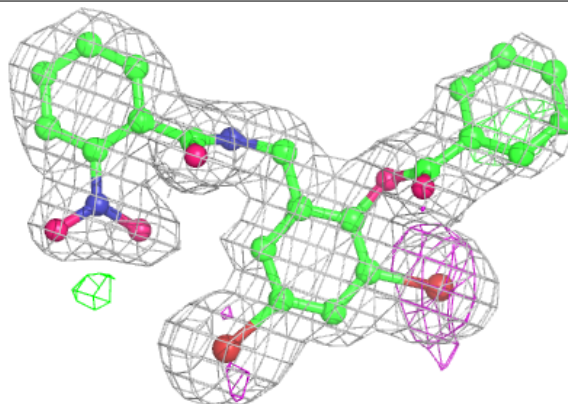
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around FXD B 300:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

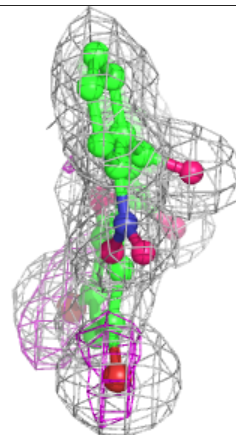
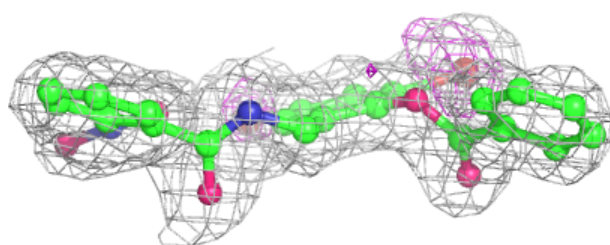
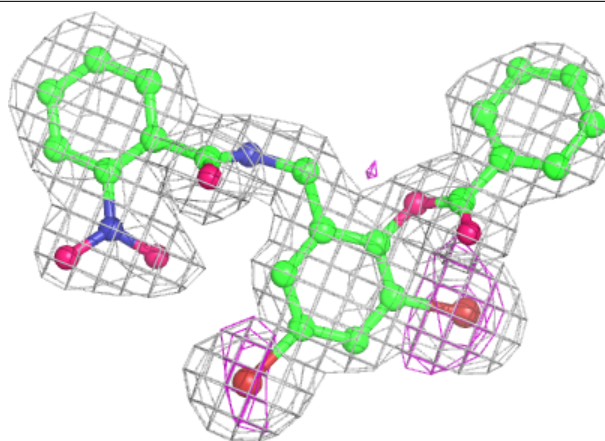
**Electron density around FXD D 300:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



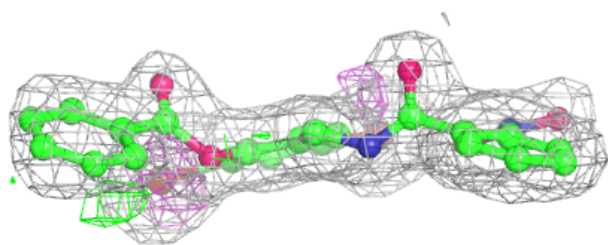
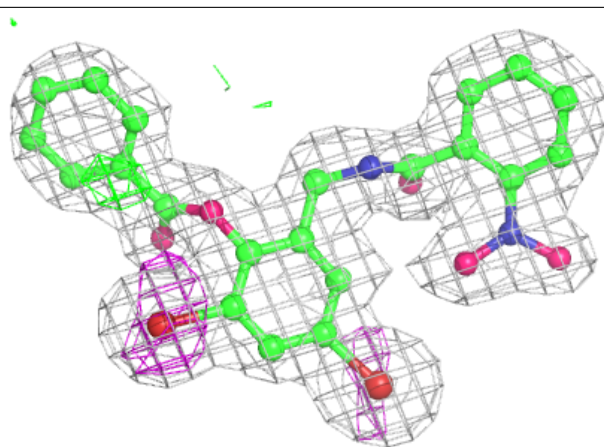
**Electron density around FXD E 300:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

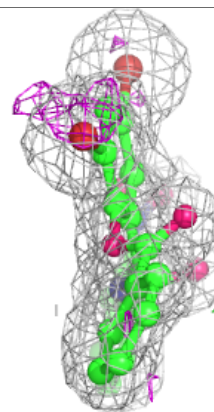
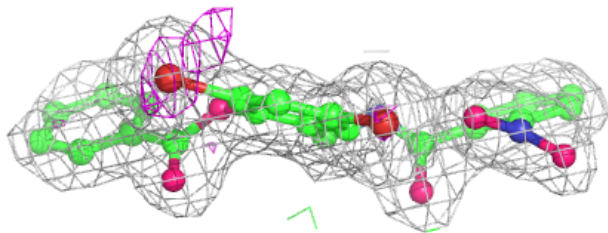
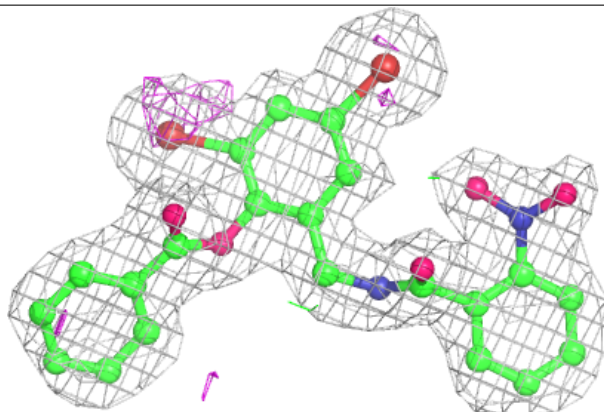


**Electron density around FXD G 300:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

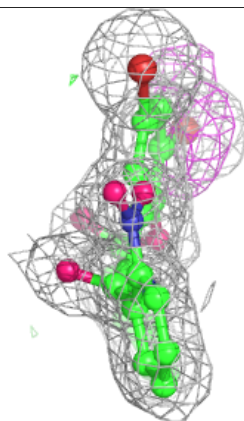
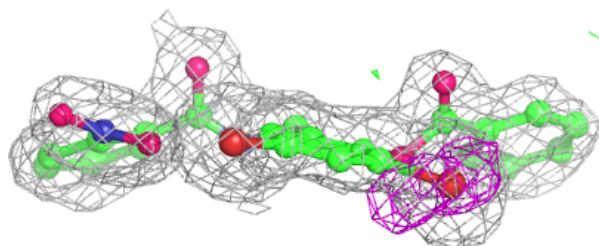
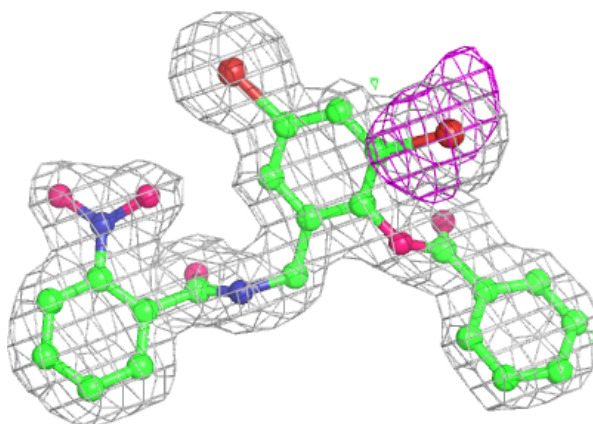
**Electron density around FXD H 300:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

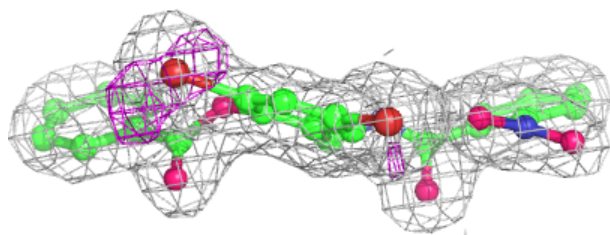
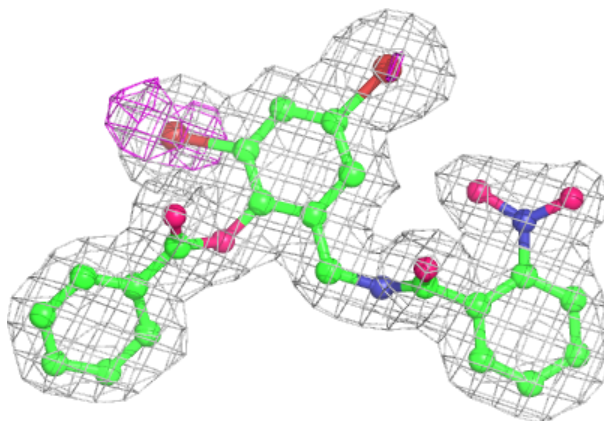


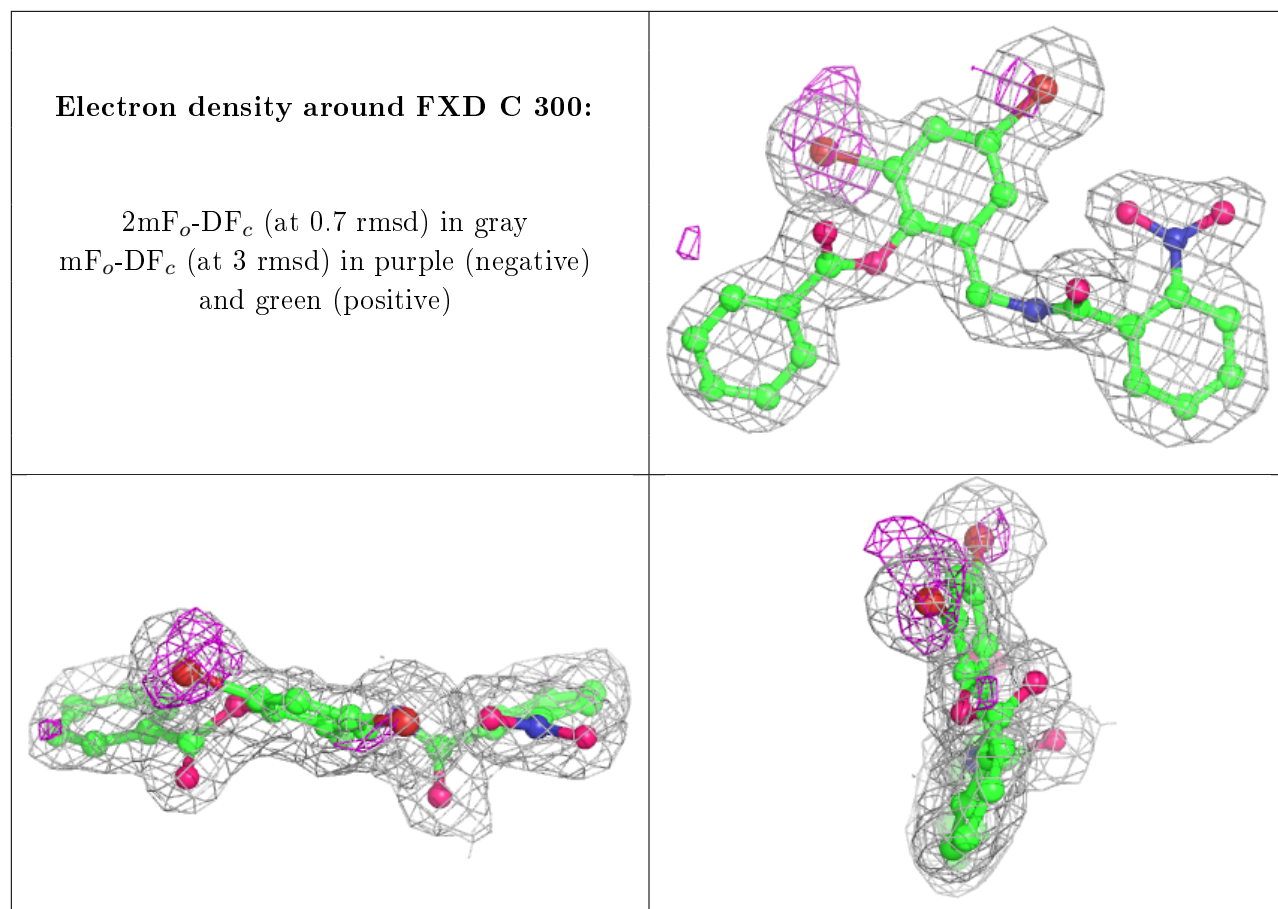
**Electron density around FXD A 300:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around FXD F 300:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.